trans-1,2-Dimethylcycloheptane

Inchi: InChI=1S/C9H18/c1-8-6-4-3-5-7-9(8)2/h8-9H,3-7H2,1-2H3/t8-,9-/m0/s1
InchiKey: CLYDEJQPKBFLJW-IUCAKERBSA-N
Formula: C9H18
SMILES: CC1CCCCCC1C
Mol. weight [g/mol]: 126.24
CAS: 13151-50-3

Physical Properties

Property code	Value	Unit	Source
gf	29.54	kJ/mol	Joback Method
hf	-201.27	kJ/mol	Joback Method
hfus	9.87	kJ/mol	Joback Method
hvap	35.92	kJ/mol	Joback Method
ie	10.31 ± 0.05	eV	NIST Webbook
ie	10.31	eV	NIST Webbook
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	941.00		NIST Webbook
tb	424.47	K	Joback Method
tc	631.20	K	Joback Method
tf	190.81	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.42	J/mol×K	424.47	Joback Method
cpg	345.35	J/mol×K	596.74	Joback Method
cpg	328.92	J/mol×K	562.29	Joback Method
cpg	311.63	J/mol×K	527.83	Joback Method
cpg	293.45	J/mol×K	493.38	Joback Method
cpg	274.39	J/mol×K	458.92	Joback Method

cpg	360.93	J/mol×K	631.20	Joback Method
dvisc	0.0002364	Pa×s	424.47	Joback Method
dvisc	0.0003181	Pa×s	385.53	Joback Method
dvisc	0.0004576	Pa×s	346.58	Joback Method
dvisc	0.0007219	Pa×s	307.64	Joback Method
dvisc	0.0012995	Pa×s	268.70	Joback Method
dvisc	0.0028552	Pa×s	229.75	Joback Method
dvisc	0.0086504	Pa×s	190.81	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13151503&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume